Supporting Information

^{1}H NMR Studies of Nickel(II) Complexes Bound to Oligonucleotides: A Novel Technique for Distinguishing the Binding Locations of Metal Complexes in DNA.

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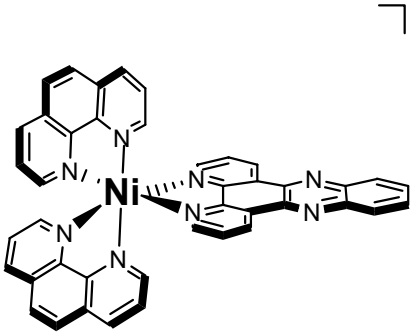
Supporting Information Available:

S1. Effects of $[Ni(phen)_2(dppz)]Cl_2$ on the ^1H NMR spectrum of $d(GTCGAC)_2$ in 90/10 H_2O/D_2O at 4 °C on a Varian Unity*PLUS*-600 NMR spectrometer. Shown is the aromatic region. The DNA sample contained 0.5 mM duplex, 5mM NaCl, 15 mM sodium phosphate, pD 7.0 in 100% D_2O. The free metal complex sample contained 0.2 mM $[Ni(phen)_2(phi)]Cl_2$ in the same buffer. The chemical shifts are relative to TMSP at 4 °C. The broadening effect was most pronounced on major groove protons like T2CH3, GIH8 and G4H8 while the minor groove protons A5H2, G1NH2 and G4NH2 remained relatively unbroadened.

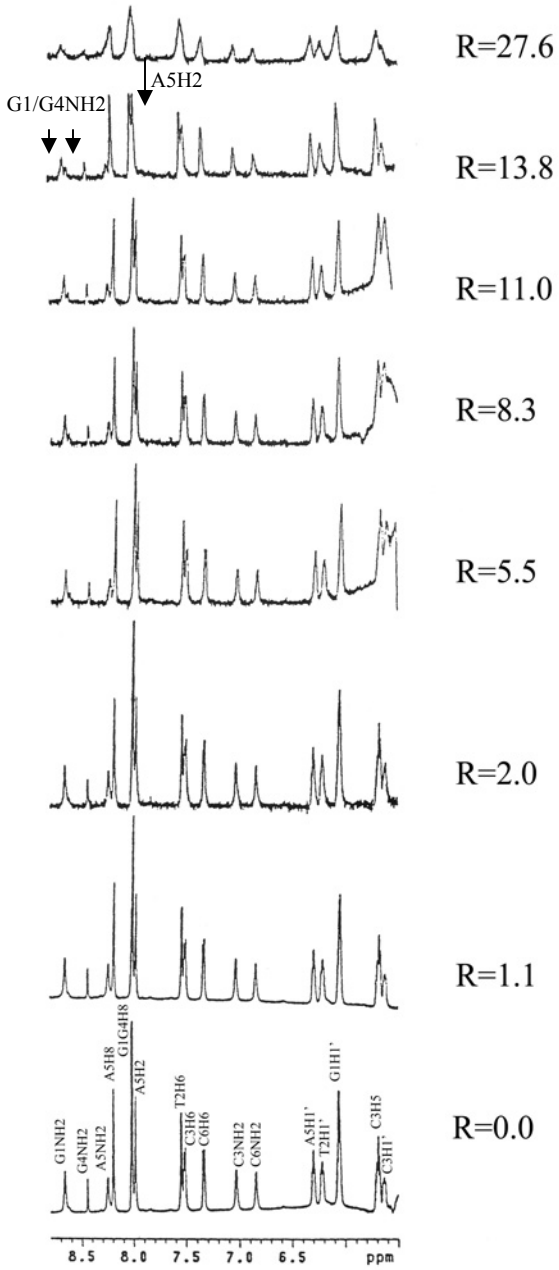
S2. Effects of $[Ni(phen)_2(phi)]Cl_2$ on the ^1H NMR spectrum of $d(GTCGAC)_2$ in D_2O at 4 °C on a Varian Unity*PLUS*-600 NMR spectrometer. Shown is the aromatic region. The DNA sample contained 0.5 mM duplex, 5 mM NaCl, 50 mM sodium phosphate, pD 7.0 in 100% D_2O. The free metal complex sample contained 0.2 mM $[Ni(phen)_2(phi)]Cl_2$ in the same buffer. The chemical shifts are relative to TMSP at 4 °C.

S3. Effects of $[Ni(phen)_2(phi)]Cl_2$ on the ^1H NMR spectrum of $d(GT\underline{GC}AC)_2$ in D_2O at 4 °C on a Varian Unity*PLUS*-600 NMR spectrometer. Shown is the aromatic region. The DNA sample contained 0.5 mM duplex, 5 mM NaCl, 50 mM sodium phosphate, pD 7.0 in 100% D_2O. The free metal complex sample contained 0.5 mM of $[Ni(phen)_2(phi)]Cl_2$ in the same buffer. The chemical shifts are relative to TMSP at 4 °C.



5'GTCGAC3'
3'CAGCTG5'

R= Metal/1000 base-pairs



R=27.6

R=13.8

R=11.0

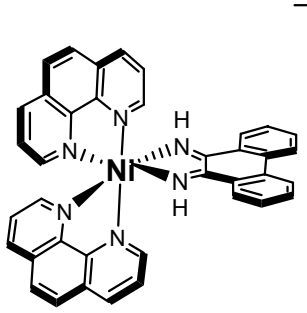
R=8.3

R=5.5

R=2.0

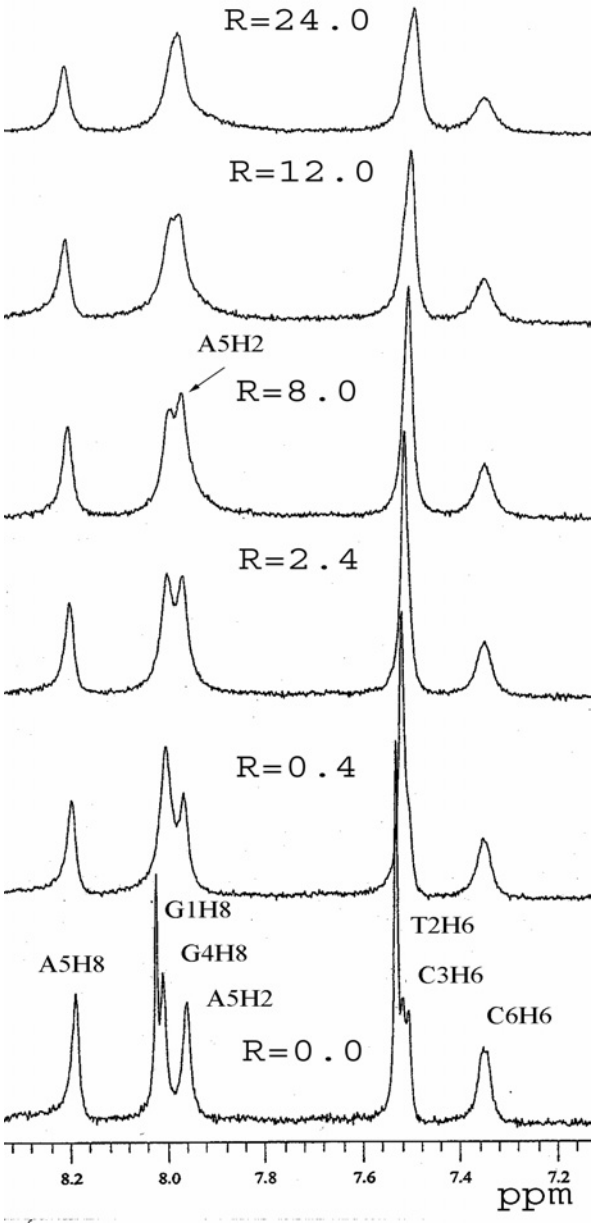
R=1.1

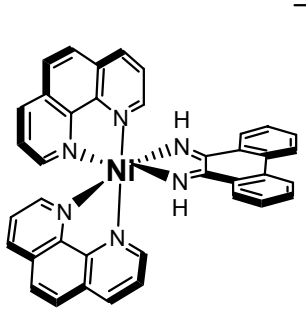
R=0.0



5'GTCGAC3'
3'CAGCTG5'

R= Metal/1000 base-pairs





5'GT<u>GC</u>AC3'
3'CA<u>CG</u>TG5'

R= Metal/1000 base-pairs